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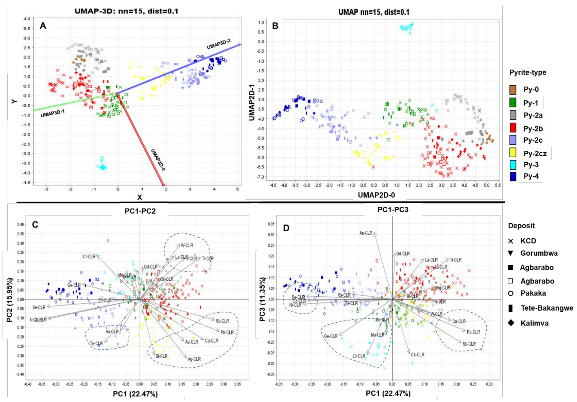

Unlocking pyrite LA-ICP-MS trace elements: the power of dimensionality reduction using synergy between UMAP, PCA and k-Means clustering

YANN MPAKA WAKU[1,2] AND BJORN VON DER HEYDEN[1]

[1]Stellenbosch University

[2]University of Kinshasa

Presenting Author: 23515635@sun.ac.za

Pyrite has gained recognition as an important indicator for deciphering the formation of mineral deposits due to its ubiquity and propensity to incorporate trace elements into its mineral structure. A comprehensive characterisation considering both the compositional and the textural properties of this sulphide mineral is crucial towards understanding the conditions that led to its formation. However, conventional methods often fail to capture the nuanced differences between pyrite samples. This study presents a dimensionality reduction-based approach to pyrite classification that reduces the dimensionality of 19-element analyses of in-situ laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) data. This novel approach incorporates the strengths of Uniform Manifold Approximation and Projection (UMAP) and Principle Component Analysis (PCA), including the unsupervised k-Means clustering to improve the visual reduction of data.

The study analysed 390 pyrite spots sourced from eight gold deposits in the world-class Kibali Gold District (northeast Democratic Republic of Congo), which had previously been classified into different generations based on textural characteristics. The dimensionality reduction algorithms suggest that these pyrite clusters into nine groupings, including py-0 (microcrystalline sooty), py-1 (fine-grained), py-2 (core-rim), py-3 (veinlet) and py-4 (euhedral free-inclusion). The new classification is around 68% different from the one done only visually and clearly shows distinct clusters. Furthermore, the principal component analysis (PCA) algorithm was performed in the centred log-ratio trace element dataset. The results highlight that the Se, Ni, Co and ±Ge, are negatively associated with PC1 and spatially occur with py-4b and py-2c, whereas Pb and Sb are positively associated with PC1.

The PC2 is positively dominated by W, Cr and V, which are spatially associated with py-0, py-1, py-2a and py-2b. Bi, Ag, Au and Cu form a negative vector group associated with the PC2 where spatially occur py-2cz. These results demonstrate the efficacy of this approach in visualising and classifying high-dimensionality data, offering a more comprehensive insight into the relationships between trace elements, texture, and morphology in different generations of pyrite. The findings of this study hold the potential to significantly enhance the accuracy of differentiating pyrite types from within various geological settings.